MST*e* NEWS

MST staff in the news

Don Brown recognized for outstanding mentoring

Don Brown (Materials Science in Radiation and Dynamics Extremes, MST-8) has received a 2019 Los Alamos Distinguished Mentor Award. Presented by the Student Programs Advisory Committee, the awards recognize outstanding performance by Lab mentors.

Brown was nominated by his current student, Tom Stockman (Finishing Manufacturing Science, Sigma-2), with support from current and previous students, including Nathan Johnson, Nicholas Bachus, and Nicholas Ferreri, and former postdoctoral researchers Maria Strantza and Eloisa Zepeda-Alarcon (all MST-8).

According to his nominators, Brown encourages his students' scientific creativity and enables them to pursue their ideas by connecting them with needed resources using his experience and networks within the material science, neutron diffraction, and additive manufacturing communities. He trusts his students with leadership roles and allows them to develop their potential by sending them to conferences and experiments conducted at other experimental facilities. He provides them with a holistic view of their research by discussing its context within the Laboratory, the Department of Energy, and the scientific community.

Brown, who has a PhD in physics from The Pennsylvania State University, leads MST-8's scattering science team. At the Los Alamos Neutron Science Center (LANSCE), the team examines mission-relevant materials under extreme environments to understand how manufacturing techniques can affect microstructure and ultimately performance. Brown develops experiments and assists researchers using the Spectrometer for Materials Research at Temperature and Stress and the High Pressure Preferred Orientation instrument as part of the LANSCE user program.

Technical contact: Don Brown

Nathan Bieberdorf receives distinguished student award

Nathan Bieberdorf (Materials Science in Radiation and Dynamics Extremes, MST-8) received a 2019 Los Alamos Distinguished Student Award. The awards, presented by the Student Programs Advisory Committee, recognize outstanding performance by Laboratory students.

Bieberdorf is a post-master's student on MST-8's Dynamic and Quasi-Static Loading team. During his nine months at the Laboratory, Bieberdorf developed

MST staff cont.

a microstructure-sensitive model that predicts how damage evolves in metals subjected to extreme environments. He quickly adapted it to address a different challenge—accurately modeling the stress around fission bubbles that form within nuclear fuels.

His results helped attract funding and spur collaboration with one power company, secure continuing DOE funding for the group's eXtreme MATerials (XMAT) program to create a robust model for designing metals, complete a milestone for the DOE's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, and establish LANL as a leader within NEAMS.

Mentor Laurent Capolungo (MST-8) nominated Bieberdorf for the award. Capolungo, with his colleagues, noted his exceptional creativity, rigor, and methodology. Bieberdorf is pursuing his PhD in materials science and engineering at the University of California, Berkeley.

Technical contact: Nathan Bieberdorf

Saryu Fensin guest edits JOM *issue*
Issue's cover highlights a column by
TMS President James Foley

Saryu Fensin (Materials Science in Radiation and Dynamic Extremes, MST-8) served as guest editor for a *JOM* section focused on materials deformation and transitions at grain boundaries. *JOM* is the journal of TMS (The Minerals, Metals & Materials Society).

Fensin and her fellow guest editors Thomas Bieler (Michigan State University), Shen Dillion (University of Illinois at Urbana-Champagne), Jian Luo (University of California, San

Diego), and Douglas Spearot (University of Florida) were chosen due to their extensive experience in understanding the mechanical behavior of materials, particularly in relation to interfaces. For the section, they selected experimental and modeling articles that studied the connection between interfaces and materials properties or that highlighted novel design approaches that improve material properties under extreme conditions. The section included an article, "Interplay between grain boundaries and radiation damage," authored by Osman El-Atwani (MST-8) and Christopher M. Barr (Sandia National Laboratories, SNL), Djamel Kaoumi (North Carolina State University), and Khalid Hattar (SNL).

The refinement or development of new materials for novel future applications relies on understanding the factors that control material properties. The ability to create materials with controlled functionality and predictable performance is the key aim of the Lab's Materials for the Future strategy.

Fensin has served on TMS's Young Professionals, Professional Development, Diversity, and Mechanical Behavior of Materials committees. She is the recipient of an AIME Robert Lansing Hardy Award, the TMS Young Leaders International Scholar—Japanese Institute of Metals Award, and the TMS Young Leaders Professional Development Award.

Reference: *JOM* 71, (2019).

Technical contact: Saryu Fensin

Christina Hanson awarded for outstanding presentation at 'Science in 3'

Christina Hanson (Engineered Materials, MST-7) was recognized as an outstanding presenter at the 2019 "Science in 3" competition. In the career development event organized by the Postdoc Program Office, Laboratory postdoctoral researchers presented their work in under three minutes to a general audience.

Presenters were judged by an external review panel on how well they engaged the audience, how clearly they communicated key concepts, and how effectively they focused and presented their ideas.

In "Putting airplanes and space shuttles on a diet," Hanson described the challenge industrial manufacturers face in producing lightweight materials that maintain important properties such as strength, durability, breathability, and specific permeability. Her presentation described research into polyimide aerogels, which have been found to have good compressibility strength at a variety of densities and can be formulated from a variety of precursors, allowing for flexibility in several properties of interest.

The issue's cover highlighted 2019 TMS President James Foley, who in an article outlined his vision for "A simple plan for a successful year." Foley is Fabrication Manufacturing Science (Sigma-1) group leader.

JOM

APRIL 2019
jom.tms.org

An official publication of The Minerals, Metals & Materials Society

MEET THE 2019 TMS PRESIDENT: James Foley Plans for Success

TMS Springer

From left: Carol Burns (Science, Technology, and Engineering, DDSTE), Kim Schultz (DARHT Physics and Pulsed Power, J-5), John Greenhall (Materials Synthesis and Integrated Devices, MPA-11), Deborah Shutt (Information Systems and Modeling, A-1), Derrick Kaseman (Bioenergy and Biome Sciences, B-11), Christina Hanson (Engineered Materials, MST-7), Eric Davis (MPA-11), and Nan Sauer (Partnerships and Pipeline Office, PPO).

MST staff cont.

Hanson received her PhD from the University of New Mexico and is mentored by Chris Hamilton and Robert Gilbertson (both MST-7).

Additional MST postdoctoral researchers presenting were
- Anjana Talapatra (Materials Science in Radiation and Dynamics Extremes, MST-8), "Materials that glow— discovering and designing new materials with machine learning,"
- Ethan Walker (MST-7), "Printing particle accelerators out of nanocomposites," and
- Eloisa Zepeda-Alarcon (MST-8), "In situ microstructural evolution of cast and wrought U6Nb under load."

Technical contact: Christina Hanson

Blaine Randolph recognized for innovation and excellence in target fabrication

Randall (Blaine) Randolph (Engineered Materials, MST-7) has received the Larry Foreman award for his substantive contributions toward innovation and excellence in target fabrication for inertial confinement fusion (ICF).

The award was presented at the recent Target Fabrication Meeting, an international gathering of experts to consider scientific, technical, and logistical challenges related to achieving ICF. This is the first time the award has been given to a machinist. Randolph shared the award with his fellow machinist Carlos Castro (Lawrence Livermore National Laboratory).

Randolph has made essential contributions to the ICF and High Energy Density Physics programs at Los Alamos for more than 30 years. He is internationally known for his unconventional and innovative machining methods, custom precision tooling, and programming. He has fabricated custom target components for pulsed power, laser, and high explosive facilities. These facilities include the Proton Radiography and Trident Laser facilities at Los Alamos, the Tandem Linear Accelerator System at Argonne National Laboratory, Nova and the National Ignition Facility at Lawrence Livermore National Laboratory, OMEGA at the University of Rochester, and Orion at the Atomic Weapons Establishment.

Blaine Randolph (right) receives the Larry Foreman Award from Target Engineering Team Leader John Oertel (both Engineered Materials, MST-7).

The award is named after the pioneering Los Alamos fusion physicist who influenced the ICF field with innovative target designs. Foreman's peers established the award, presenting it every year since 1999. Previous Los Alamos recipients include Pete Gobby, James Hoffer, and Robert Day.

Technical contact: Blaine Randolph

Rachel Flanagan electrifies with five-minute 'Lightning Talk'

Rachel Flanagan (Materials Science in Radiation and Dynamics Extremes, MST-8) recently took to the stage at the J. R. Oppenheimer Center to present her work as part of "Lightning Talks." In the TEDx-inspired event hosted by the Student Programs Office, students had five minutes to present their research to a broad audience.
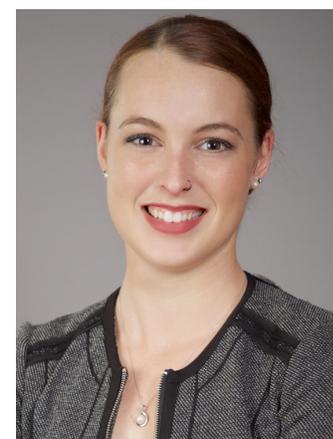
In "An atom's perspective of shock," Flanagan discussed her research into using molecular dynamics simulations to understand the behavior of individual atoms as they undergo shock. The ultimate goal of her research is the ability to predict the strength and failure of any material. Flanagan, a student in the Mechanical and Aerospace Engineering Department at the University of California, San Diego, is mentored by Saryu Fensin (MST-8).

Technical contact: Rachel Flanagan

New surface science instrumentation for understanding the reactivity of plutonium

Students and early-career staff eager to gain experience with surface science instrumentation fully configured for studying radioactive materials have the opportunity to do so at the Plutonium Surface Science Laboratory in the Lab's Target Fabrication Facility. Scientists can study plutonium more easily at this facility, which does not require the extensive training needed to work in the Plutonium Facility.

In *Actinide Research Quarterly*, Sarah Hernandez (Nuclear Materials Science, MST-16) highlighted the laboratory and the results of her research using its capabilities. In many cases, she wrote, the lab's surface analytical techniques have never been applied to plutonium surfaces and are providing new insights into understanding plutonium reactivity.

Hernandez, who received her PhD in physics from the University of Texas at Arlington, was a Seaborg Institute Postdoctoral Research Fellow before becoming an MST-16 staff scientist. Her studies include the oxidation and corrosion of plutonium and aging of plutonium using density functional theory methods.

Hernandez and collaborators used time-of-flight secondary ion mass spectrometry (ToF-SIMS) to detect negative and positive secondary ion fragments, which provided insight into the surface species that might exist. Their results reveal that gallium is located at the surface of gallium-stabilized delta-plutonium and is reactive to oxygen exposure. They showed that gallium is also reactive to other environmental gas exposures, such as water vapor. Further studies are needed to fully understand the PuHx fragments, and there are future plans to investigate a deuterium-loaded, gallium-stabilized delta-plutonium sample to determine the source of the hydrogen. As a whole, the suite of experimental surface science instruments within the Plutonium Surface Science Laboratory delivers a powerful ability to explore the oxidation and corrosion of plutonium surfaces from a multitude of perspectives.

Actinide Research Quarterly is published by Los Alamos National Laboratory and is a publication of the Glenn T. Seaborg Institute for Transactinium Science, a part of the National Security Education Center. The publication highlights research in actinide science in such areas as process chemistry, metallurgy, surface and separation sciences, atomic and molecular sciences, actinide ceramics and nuclear fuels, characterization, spectroscopy, analysis, and manufacturing technologies.

Reference: "New surface science instrumentation for understanding the reactivity of plutonium," *Actinide Research Quarterly*, 1, 33 (2019).

Technical contact: Sarah Hernandez

Machine-learning scintillator model finds new predictors of light yield

Los Alamos scientists have combined the Lab's expertise in radiation detection with the power of its high-performance computing clusters to design a two-pronged, machine-learning-based approach to scintillator design. In a feat of machine-learning techniques, the researchers used only a limited set of data to train their computer model and identified previously unknown characteristics that contribute to scintillator performance. The research was selected as the June finalist for the *Journal of Materials Science* Robert

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Materials — Computation and/or Experiments — **Properties**

Conventional Route

Data-enabled Route

Fingerprinting — Statistical Learning
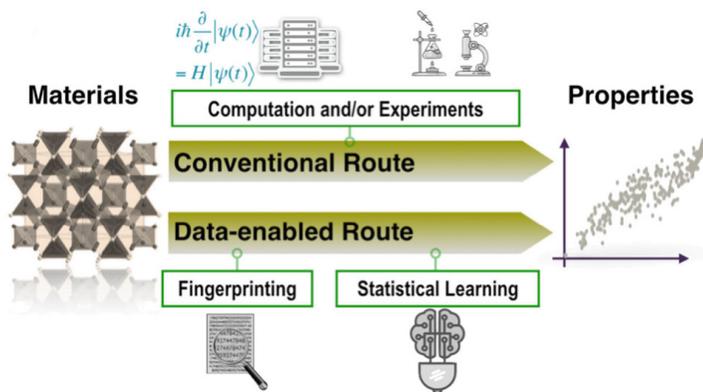
The conventional route of the scientific process is centered on experts devising experiments or developing computation methods based on their understanding of physics. The data-enabled route applies statistical models to a set of established features, or fingerprints, without incorporating scientific knowledge. In this work, the authors combined the conventional and data-enabled routes to find fingerprints that are predictive of experimental performance and predict future scintillator materials.

Machine-learning cont.

W. Cahn Best Paper Prize. One article is selected each month as a Cahn Prize finalist, with the award presented in December.

Scintillators—materials that fluoresce with sharp pulses of light when excited by ionizing radiation—are used to detect radiation, including light, for a variety of scientific, medical, and industrial applications. For example, new, bright, fast scintillators will image the high-repetition-rate experiments in extreme environments proposed to fulfill the DOE's currently unmet Dynamic Mesoscale Material Science Capability.

Historically, developing a new scintillator material has been a resource-intensive process of trial and error, taking nearly a decade from discovery to deployment. Because the crystals used to make scintillators have many well-defined characteristics—including chemistry, dopant concentration, bandgap, crystal structure, and grain size—machine learning could be a good candidate for scintillator design. However, most machine learning paradigms require hundreds or thousands of samples to train the computer, and few scintillator materials exist that can serve as the basis for such training.

To allow the computer to learn from a limited set of data, the authors built on their previously developed technique, which incorporates known physics phenomena into the computer's learning process. With this new method, they trained the learning algorithm on a carefully chosen set of only 25 lanthanide-doped scintillator materials for which there was reliable data on desirable characteristics, such as the material's light output and decay time. Using this small set, they identified relevant features for predicting light output and decay time and determined the level of accuracy for these predictions. Their machine-learning technique identified characteristics that had not previously been directly linked to scintillation. It found that the lattice component of the dielectric constant is a highly relevant predictor for light yield, irrespective of the specific chemistry of the compound.

Funding for this technology maturation work came from the Laboratory's MaRIE project (LANL Capture Manager Cris Barnes) through Campaign 2 (LANL Program Manager

Dana Dattelbaum). This work supports the Laboratory's Nuclear Deterrence mission and its Materials for the Future and Nuclear and Particle Futures science pillars by enabling the informed design of materials for future radiation detection devices. It supports the Information, Science, and Technology science pillar by using Los Alamos's high-performance computational capabilities to accelerate the predictive capability of the scientific method.

Researchers: Ghanshyam Pilania and Xiang-Yang Liu (Materials Science in Radiation and Dynamics Extremes, MST-8) and Zhehui Wang (Subatomic Physics, P-25).

Reference: "Data-enabled structure–property mappings for lanthanide-activated inorganic scintillators," *J Mater Sci* 54, 8361-8380 (2019).

Technical contact: Ghanshyam Pilania

Evidence that electrons can help study materials under extreme conditions

Researchers in MST and Engineering Technology and Design (E-DO) divisions, in collaboration with the Naval Research Laboratory (NRL), have made a first step in demonstrating that electrons can be used as surrogates for rapid heating of materials. This was accomplished using Gamble II—a pulsed-power electron beam line at NRL.

Built in 1970, Gamble II was the first water-dielectric machine in the West. Now, it is commonly used as an inexpensive "pre-test" for novel materials. Many successful Gamble II experiments proceed to more expensive testing at the National Ignition Facility at Lawrence Livermore National Laboratory or the Z Pulsed Power Facility at Sandia National Laboratories.

The most recent use of Gamble II illustrated that electron beam irradiation can imitate extreme conditions for materials and those results can be quantified. The Los Alamos and NRL researchers irradiated foam material and measured the
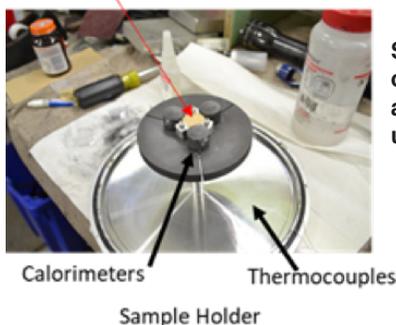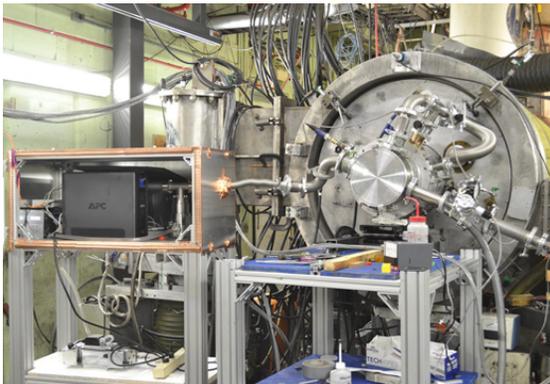
Sample holder and layout of the Gamble II beam line and residual gas analyzer used for the experiments.

Evidence cont.

gas decomposition products with a residual gas analyzer. The residual gas spectra showed evidence of the chemical changes the sample underwent and visual inspection of the samples showed the physical damage (e.g., charring) caused by the electron beam irradiation.

This was the first time in situ information was acquired on the chemical and physical changes that materials undergo under extreme conditions. Ex situ characterization of the materials before and after electron beam irradiation demonstrated significant material property changes, which is in agreement with the residual gas data obtained during the experiments. Preliminary density functional theory studies of the fragmentation of this material was also in agreement with the data: multiple bonds break at once, with carbon monoxide and ethylene being emitted first during rapid heating.

This evidence will allow more materials under extreme conditions to be studied and understood. This research was recently submitted for peer review for the upcoming 2020 Weapons Engineering Symposium at LANL.

Campaign 7 (LANL Program Manager Steve McCready) funded this research, which was performed at LANL and NRL. LANL scientists and engineers performed material characterization before and after electron irradiation. This work supports the Laboratory's Nuclear Deterrence mission and Materials for the Future science pillar.

Researchers: Loren I. Espada Castillo (Engineered Materials, MST-7), Erwin Schwegler (Advanced Engineering Analysis, E-13), Martin Perraglio (Mechanical and Thermal Engineering, E-1), Isaac Herrera and Paul Peterson (both MST-7), Kin Lam (E-13), and David Hinshelwood (NRL).

Technical contact: Loren I. Espada Castillo

HeadsUP!

Watch out for wildlife!

With the advent of fall weather it's important to be aware of the potential for increased wildlife activity on our roadways in the early mornings and evenings.

- Slow down: The most important way to avoid collisions with wildlife is to slow down and observe the speed limit.
- Use your eyes: Avoid a collision by keeping your eyes on the road.
- Be mindful of peak areas and times: Be on your highest alert at dusk and dawn, when many animals are most active.
- Don't tailgate: Keep a safe distance between you and the car in front of you to avoid any unnecessary accidents.
- Use your brights: Your high-beam lights are there for a reason, don't be afraid to use them.
- Remember deer and elk travel in herds: When you spot one deer or elk crossing the road, another is likely to be right behind.

Celebrating service

Congratulations to the following MST Division employees celebrating recent service anniversaries:

Kevin Graham, MST-16..35 years
Cheng Liu, MST-8...25 years
Randy Sandoval, MST-16..20 years
Dali Yang, MST-7..20 years
Monica Roybal, MST-DO...15 years
Jay Jackson, MST-16 ....15 years
Darrin Byler, MST-8 ....15 years
Tana Cardenas, MST-7..10 years
Anthony Sanchez, MST-7..10 years
Christopher Hamilton, MST-7 ....10 years
Megan Espinoza, MST-8 ....5 years
Daniel Olive, MST-16..5 years

MST e NEWS

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